Tetrachlorophthalic acid 632-58-6 | DTXSID6060896

Model Performance

Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 3.91e-09 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.08e-01

Confidence level: 3.24e-01

Nearest Neighbors from the Training Set

Image not found

p,p'-DDE

Measured: 4.46e-11 Predicted: 2.89e-06 Image not found

Pirimiphos-ethyl Measured: 2.00e-06 Predicted: 2.79e-05 Image not found

2,4-Dinitrotoluene Measured: 2.21e-08 Predicted: 2.66e-04

Image not found

MCPB ethyl

Measured: 7.50e-10 Predicted: 1.69e-05 Image not found

cis-Nonachlordane Measured: 1.20e-09 Predicted: 2.30e-06